ENERGY STATES AT THE INTERFACE OF TWO SEMI-INFINITE ONE-DIMENSIONAL CRYSTALS

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ABSTRACT. Localized energy levels are computed, by the scattering matrix method of Saxon and Hutner (1949), at the interface of two similar semi-infinite crystals with adsorbed gas at the interface. First, the calculations have been made for a clean interface and then for an impurity atom at the interface The results show the existence of localized states at certain potential strength of the adsorbed gas Some experimental evidence of the theoretical results are given.

INTRODUCTION

Tamm (1932) showed the existence of localised energy levels at the free surface of a one dimensional semi-infinite crystal. Since then several authors have calculated surface energy levels by various methods. Shockley (1939), and Aerts (1960) calculated surface energy levels on the assumption that the potential of the boundary atom shows a symmetric behaviour. Aerts further extended the case to a surface contaminated by an adsorbed impurity atom. On assuming this kind of potential, the results obtained by Aerts conform to the experimental observations

In this paper, the electronic energy states localised at the interface of two semi-infinite crystals with adsorbed gas layer at the interface, are computed Aerts (1960) has shown that the interface between two crystals is a kind of imperfection, which gives rise to energy state and thus plays a great role in its electrical behaviour. It is well established that the electrical conductivity of both semiconducting crystals and films are strongly dependent on the adsorbed gas. When films of a substance are deposited on a substrate, we have adsorbed gas at the interface of two crystallites of identical nature. The presence of an impurity may also be possible at the interface of identical crystallites. We propose to investigate the energy-states in the above mentioned systems A simple method based on the work of Saxon and Hutner (1949) has been followed.

THE CRYSTAL MODEL AND THEORY

Since the essential features of the problem would remain same, a simplified model of two semi-infinite crystals, of identical nature in contact is considered. The semi-infinite monatomic lattice has the same spacing on both sides. Let

U be the atomic potential Due to the adsorbed gas at the interface the surface atoms may be assumed to have the potential strength $U+U_1$. Let the interface potential be $U+U_2$. A graphical representation of the crystal model is given in Fig 1.

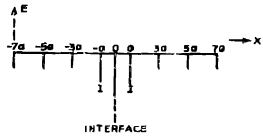

Fig 1 Graphical representation of the crystal model with adsorbed impurity (1) at the interface.

Choosing the origin of the co-ordinate system at the interface, the atoms of the R H S are localized at the points with abscissa $x = (2n+1)a$ and those of L.H.S. are localised at the points $x = -(2n+1)a$, n being a positive integer.

On the R H.S the potential energy is of the form

$$-eV_1 = \left(\frac{au\hbar^2}{m}\right) \sum_0^\infty \delta[x-(2n+1)a] + \frac{au_1\hbar^2}{m}\delta(x-a) \qquad (1)$$

and on the L H S. the potential energy is of the form

$$-eV_2 = \left(\frac{au\hbar^2}{m}\right) \sum_0^\infty \delta[x+(2n+1)a] + \frac{au_1\hbar^2}{m}\delta(x+a) \qquad (2)$$

The waves propagating from either side will undergo scattering by the combined disturbances, first at the absorbed impurity atom, then at the interface and again at the adsorbed impurity atom Following Saxon and Hutner's method, the M-matrix associated with the three combined disturbances may be given by

$$M = (R_2)(Q_2)(R_{21})(Q_1)(R_1) \qquad .. \quad (3)$$

The matrix (R_2) is associated with the adsorbed impurity situated at $x = a$. It is

$$R_2 = \begin{vmatrix} 1+i\tan\theta & i\tan\theta \\ -i\tan\theta & 1-i\tan\theta \end{vmatrix} \qquad (4)$$

where,

$$\tan\theta = \frac{au_1}{\chi}\frac{\sin 2\psi a}{\sin 2\mu a} \qquad (5)$$

where μ is the wave vector and $\chi^2 = \frac{2mE}{\hbar^2}$, E being the electron energy in the crystal.

(Q_2) is the translation matrix for $x = a$ to $x = 0$ and is of the form

$$Q_2 = \begin{vmatrix} e^{i\mu a} & 0 \\ 0 & -e^{i\mu a} \end{vmatrix} \quad \ldots \quad (6)$$

The matrix (R_{12}), associated with the disturbance at the interface potential, is given by

$$R_{12} = \begin{vmatrix} 1 - \frac{iau_2 \sin \chi a}{2\chi \sin \mu a} & -\frac{iau_2 \sin \chi a}{2\chi \sin \mu a} \\ \frac{au_2 \sin \chi a}{2\chi \sin \mu a} & 1 + \frac{au_2 \sin \chi a}{2\chi \sin \mu a} \end{vmatrix} \quad \ldots \quad (7)$$

Q_1 is the translation matrix for $x = 0$ to $x = -a$ and is of the form

$$Q_1 = \begin{vmatrix} e^{i\mu a} & 0 \\ 0 & e^{-i\mu a} \end{vmatrix} \quad \ldots \quad (8)$$

The matrix (R_1) is associated with adsorbed impurity situated at $x = -a$ and it is

$$R_1 = \begin{vmatrix} 1+i\tan\theta & i\tan\theta \\ i\tan\theta & 1-i\tan\theta \end{vmatrix} \quad \ldots \quad (9)$$

Writing $\tan\theta = A$, $e^{i\mu a} = B$ and $\frac{au_2 \sin \chi a}{2\chi \sin \mu a} = C$

and then substituting the values of (R_2), (Q_2), (R_{12}), (Q_1) and R_1 in equation (3), we have

$$M = \begin{vmatrix} 1+iA & iA & B & 0 & 1-ic & -ic & B & 0 \\ -iA & 1-iA & 0 & B & ic & 1+ic & 0 & B \end{vmatrix} \begin{vmatrix} 1+iA & iA \\ -iA & 1-iA \end{vmatrix} \quad \ldots \quad (10)$$

The localized energy levels at the interface are determined by the conditions

$$M_{22} = 0; \quad \mu = \frac{n\pi}{2a} + i\xi, \quad \xi > 0 \quad (11)$$

Using second and third conditions of equation (11), the appropriate Kronig and Penny relation can be written as

$$(-1)^n \, ch\, 2a\,\xi = \cos 2a\chi + \left(\frac{au}{\chi}\right) \sin 2a\chi \quad \ldots \quad (12)$$

The matrix element M_{22} as obtained from equation (10) is given by

$$\begin{aligned} M_{22} = {} & \tan^2\theta[2i\,(\sin\mu a - c\cos\mu a) + c] \\ & -2\tan\theta\,[i(1+ic)e^{-2i\mu a} + c] \\ & +(1+ic)e^{-2i\mu a} \end{aligned} \quad \ldots \quad (13)$$

Using the first condition of eq. (11), the two values of tan θ obtained as a solution of the quadratic Eq. (13), are given by

$$\tan\theta = \frac{\left(i\sin\mu a - \frac{au_2}{\chi}\tan\chi a\cos\mu a\right)(1-2\cos^2\mu a - 2i\sin\mu a\cos\mu a) \pm i\sin\mu a - \frac{iu_2}{\chi}\tan\chi a\cos\mu a}{2i\left[2i\sin^2\mu a\cos\mu a - \frac{au_2}{\chi}\tan\chi a\cos\mu a(1-2\sin^2\mu a) - \frac{iu_2}{\chi}\tan\chi a\cos\mu a\right]} \quad \ldots (14)$$

Putting second and third conditions of equation (11) in equation (14) and taking negative sign, we obtain

$$\tan\theta_1 = \frac{i\left[i(1+ch\,2a\xi)^{\frac{1}{2}} - \frac{au_2}{\chi}\tan\chi a(1-ch\,2a\xi)^{\frac{1}{2}}\right][(1-ch\,2a\xi)^{\frac{1}{2}} + i(1+ch\,2a\xi)^{\frac{1}{2}}]}{2\left(1+\frac{au_2}{\chi}\tan\chi a\right)(1+ch\,2a\xi)} \quad \ldots (15)$$

To obtain the energy states within the first forbidden gap we take $n = 1$ in equation (12) and by eliminating ξ between (12) and (15), we get

$$\tan\theta_1 = \frac{i/2\left[i\left(1-\frac{aU_2}{\chi}\cot a\chi\right)^{\frac{1}{2}} - \frac{au_2}{\chi}\tan a\chi\left(\cot^2 a\chi + \frac{aU}{\chi}\cot a\chi\right)^{\frac{1}{2}}\right]}{\left[\left(\cot^2 a\chi + \frac{aU}{\chi}\cos a\chi\right)^{\frac{1}{2}} + i\left(1-\frac{aU}{\chi}\cot a\chi\right)^{\frac{1}{2}}\right]} \Bigg/ \left(1+\frac{aU_2}{\chi}\tan a\chi\right)\left(1-\frac{aU}{\chi}\cot a\chi\right) \quad (16)$$

Substituting the value of tan θ_1 as in equation (5) in (16) we have

$$X_1 = \frac{V\left[1-\frac{Z^2}{V^2}+\frac{2Z}{V}\cot\pi V\right]^{\frac{1}{2}}}{2\left[1+\frac{Y}{V}\cot\pi V/2\right]\left[1-\frac{Z}{V}\cot\frac{\pi V}{2}\right]}$$

$$\left[i\left(1-\frac{Z}{V}\cot\frac{\pi V}{2}\right)\left(1+\frac{Z}{V\cot\frac{\pi V}{2}}\right)^{\frac{1}{2}}\right.$$

$$\left.\left(\cot\frac{\pi V}{2}-\frac{Y}{V}\right) - \frac{Y}{V}\cot\frac{\pi V}{2}\left(1-\frac{Z}{V\cot\frac{\pi V}{2}}\right)\right.$$

$$\left.-\left(1-\frac{Z}{V}\cot\frac{\pi V}{2}\right)\right] \quad (17)$$

where $X_1 = \frac{2a^2}{\pi} U_1$, $Y = \frac{2a^2}{\pi} U_2$; $Z = \frac{2a^2}{\pi} U$ and $V = \frac{2a}{\pi} \chi$ ... (17)

Now taking the positive sign in equation (14) for the second solution of $\tan \theta$, we similarly obtain

$$X_2 = -X_1 + \frac{V}{\sin(\pi V) + \frac{2Y}{V} \sin^2\left(\frac{\pi V}{2}\right)} \quad \ldots (18)$$

Equations (17) and (18) are rather involved in V, therefore, it is difficult to calculate the energy values directly for different values of x, i.e. different types of

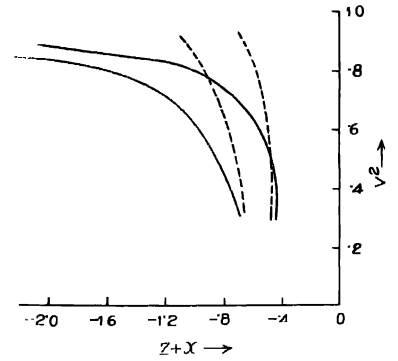

Fig. 2

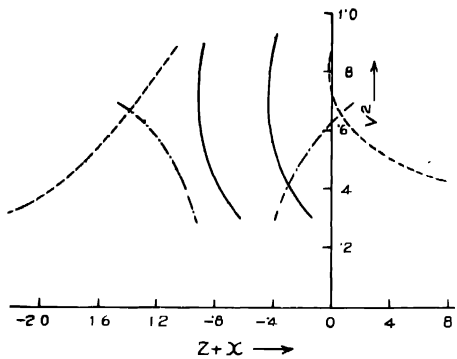

Fig 3 Solutions of the equations (17) and (18)
——— for Z = −½, Y = −1
. . for Z = −½, Y = −½
—o—o—for Z = −½, Y = 0

adsorbed gas. Hence, a assuming reasonable values of V, X_1 and X_2 have been calculated with the help of equations (17) and (18) It is thus possible to have same energy for different nature of adsorbed gas.

RESULTS AND DISCUSSION

The plots in Figs. 2 and 3 represent the results of our calculations. It should be mentioned that only the solutions that have a physical meaning are plotted Fig 2 represents the solutions for a definite value of atomic potential Z. and positive values of interface potential Y; Fig. 3 shows the solutions for a definite value of atomic potential Z with zero and negative values of interface potential Y. For positive values of Y one finds the localized energy levels at the interface when there is only adsorbed gas at the clean interface of two crystallites of identical nature and for negative values of Y there are adsorbed gas and also an impurity at the interface The plots are interrupted at certain values of V because we have restricted the calculations to the first forbidden gap.

The family of curves in Figs. 2 and 3 can in general be explained if we consider that when the potential strength of the adsorbed impurity is smaller than that of the bulk, an electron can escape more easily because it is more loosely bound and there is possibility of larger interaction with the neighbouring atomic potentials. On the contrary when the potential strength of adsorbed impurity is deeper than that of the bulk, the electron is more tightly bound to the impurity and the possibility of interaction with the neighbouring atomic potential decreases. It is, however, not possible to explain every detail of the curves only on the above considerations. It is striking to note that the energy levels move towards the conduction, creating degenerate levels near the conduction band as the impurity potentials become deeper. This means the creation of n-type levels by highly p-type impurities when they are consecutively placed in the atomic lattice or are in close proximity. It was experimentally observed by Ghosh (1960) that there is a possible existence of n-type regions in the films deposited from highly p-type tellurium The existence of n-type tellurium as such is not found, but it appears from the above discussion that an n-type region is possible in a film deposited from highly p-type materials at places where there is an accumulation of impurity atoms or a highly p-type gas adsorbed at the interface of two crystallites.

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